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Modeling anisotropic diffusion using a departure from isotropy approach

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ABSTRACT

There are a large number of finite volume solvers available for solution of *isotropic* diffusion equation. This article presents an approach of adapting these solvers to solve *anisotropic* diffusion equations. The formulation works by decomposing the diffusive flux into a component associated with isotropic diffusion and another component associated with *departure* from isotropic diffusion. This results in an *isotropic* diffusion equation with additional terms to account for the anisotropic effect. These additional terms are treated using a deferred correction approach and coupled via an iterative procedure. The presented approach is validated against various diffusion problems in anisotropic media with known analytical or numerical solutions. Although demonstrated for two-dimensional problems, extension of the present approach to three-dimensional problems is straight forward. Other than the finite volume method, this approach can be applied to any discretization method.

1. Introduction

Isotropic diffusion equation governs a very wide range of physical processes occurring in isotropic media, including heat, mass and momentum transfers. Most media encountered in physical and engineering applications are however anisotropic in nature. For these media, the directional dependence of their diffusion coefficients must be accounted for. This equation needs to be further generalized by introducing the generalized Fick's law [1,2] with an anisotropic diffusion coefficient, and thus forming the anisotropic diffusion equation with additional mixed derivative terms. These mixed derivative terms characterize the more complicated interactions in the physical process originated from the anisotropy of the media under investigation. Isotropic diffusion equation is therefore a very special limiting case of an anisotropic diffusion equation.

Anisotropic diffusion equation arises in very diverse physical processes. Diffusion of water vapors, organic vapors and gases in soil, diffusion of nutrients away from fertilizer granules towards plant roots in soil and diffusion of contaminants within subsurface geological formations are examples of solutal diffusion transport in porous media [3–5]. The structure of these naturally occurring porous media is highly irregular in terms of the pore distribution with respect to both size and shape. Given the anisotropy (and the heterogeneity) of the media, such diffusion processes can be appropriately modeled with an anisotropic diffusion equation. Besides, the generalized Darcy's law coupled with the continuity equation for modeling fluid flow in anisotropic heterogeneous porous media, e.g. subsurface geological formations, gives rise to a similar anisotropic diffusion equation in terms of the fluid pressure [6,7]. Heat transfer in structural materials, e.g. wood and laminated metal sheets, and crystals is another flourishing field where anisotropic diffusion equation is generally applied [8–10]. Interestingly, in the recent years, anisotropic diffusion equation finds its application in the field of imaging, e.g. diffusion-tensor magnetic resonance imaging [11] and more generally PDE-based anisotropic diffusion filters [12–14].

From a historical point of view, solutions of isotropic diffusion equation were attempted much earlier than that of anisotropic diffusion equation. Isotropic diffusion equation has a lucidly simpler mathematical structure and therefore is more amenable to both analytical and numerical approaches. Some of these developed numerical approaches, e.g. based on the finite difference (FD), finite volume (FV), finite element (FE), boundary element (BE) methods and fast Poisson solver [15–19], are now well established and implemented routinely as standard solvers, at least for simple geometrical configurations. For more complicated geometrical configurations, numerical solution implemented on unstructured mesh is still being actively pursued for example in the recent work of [20]. Driven by the pressing needs of the above mentioned practical applications involving anisotropic media, these methods are then

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Nomenclature

A	surface area of a control volume
$\|E\|_2$	root mean square norm error
$\|E\|_\infty$	maximum norm of error
h	refinement ratio
$\bar{\bar{I}}$	identity matrix
k	thermal conductivity
$\vec{q}$	diffusive flux
$\vec{q}_D$	departure from isotropic component of the diffusive flux
$\vec{q}_{\max}$	isotropic component of the diffusive flux
Q_{gen}	volumetric heat generation
R	rotational matrix
S	source term
S_D	source term due to departure from isotropic
T	temperature
$\vec{x}$	position vector
x	coordinate axis
y	coordinate axis

Greek letters

ΔV	volume
ΔA	surface area
ε	degree of anisotropic
ϕ	transported quantity
$\bar{\bar{\Gamma}}$	diffusion coefficient
$\Gamma_{\max}$	isotropic component of the diffusion coefficient
$\bar{\bar{\Gamma}}_D$	departure from isotropic component of the diffusion coefficient
Ω	domain of interest
$\partial\Omega^q$	boundary with prescribed flux
$\partial\Omega^\phi$	boundary with prescribed ϕ
θ	orientation of the principal directions

Superscript

m	current iteration
P	prescribed value
$*$	principal directions

Subscript

ave	average
B	boundary control volume
n	normal
P	control volume P

generalized to anisotropic diffusion equation. Such generalizations require careful consideration of the discretization procedure that gives proper discretization of the diffusion terms.

The applications of FD method for various anisotropic diffusion problems were made in [7,21,22]. In [21], the coordinate system is realigned with the principal direction of the anisotropic diffusion coefficient so that the cross derivative terms vanish. This approach is however difficult to be generalized for heterogeneous media where the principal direction changes spatially. Of particular interest is the improvement made by the introduction of mimetic approach [23,24]. Mimetic approach incorporates the essential property of conservation during the discretization procedure and gives locally conservative discretization equations. The FV method was also extended and employed in the works of [25–27]. For FV method, an accurate approximation of the flux at the control volume face remains one of the challenges. Flux-continuity across the control volume faces has been given extra attention to produce locally conservative schemes [27–29]. Matrix- [30] and flux-splitting [31] approaches were formulated for the FV method on structured and unstructured mesh. These approaches employ a deferred correction approach so that the coefficient matrix and the flux vector retain similar forms as those resulted from simple diffusion problems. The FE method was employed in [32,33] with proper modifications in the treatment of the additional mixed derivative terms. One notable effort that increase the method's accuracy is incorporation of the adaptive mesh approach into the framework of a FE method where the underlying mesh adapts dynamically during the solution process was developed [34]. This adaptive mesh approach although costly gives excellent results with much lesser numerical smearing for diffusion in highly anisotropic media. Extension and applications of the BE method in various problems involving conduction heat transfer, fluid flow in porous media and structural problem of an elliptical bar under torsion have been demonstrated in [35,36]. It should be mentioned that some of these extensions require intricate discretization procedure and therefore not straight forward to implement numerically.

Here in this article, an alternative approach that adapts the existing solvers for isotropic diffusion equation to solve anisotropic diffusion equation is presented. In this approach, the diffusive flux is decomposed into a component associated with isotropic diffusion and another component associated with *departure* from isotropic diffusion. This decomposition transforms an anisotropic diffusion equation into the form of an isotropic diffusion equation with additional terms to account for the anisotropic effect. These additional terms are treated using a deferred correction approach and coupled via an iterative procedure. The advantage of the decomposition approach proposed here is that it allows existing solvers for isotropic problems to be extended easily to anisotropic diffusion problems (at least for orthogonal coordinate systems). The main contribution of this proposed approach is the simplicity it offers in the implementation of such an extension. It just requires an additional subroutine be written to evaluate the departure from isotropic term and called from the original solver. No other modification on the original code of the solver is required.

It should be noted that different deferred correction approaches have been proposed for the solution of anisotropic diffusion problems. In the flux-splitting approach at the flux level [30,31], the flux is split into the form of a leading two-point flux and additional cross-diffusion terms. The leading two-point flux term is approximated implicitly but the remainder flux term is treated explicitly and coupled iteratively. With this, the standard five-point (seven-point) stencil is preserved for two-dimensional (three-dimensional) problems. For flux-splitting at the matrix level [30,31], the coefficient matrix in the system of linear equations is effectively decomposed into a penta-diagonal matrix and a residual matrix. The penta-diagonal matrix is in the similar form that would be obtained by discretizing a simple diffusion equation. In the work of [25], only the cross diffusion terms are approximated explicitly via a deferred correction approach and coupled iteratively. Adaptation of these approaches into existing solvers for isotropic diffusion problems requires more modifications on the original code for the case where the diagonal components of the diffusion coefficient are different.

The remaining of the article is separated into five sections. A description of the problem is given in Section 2. Section 3 is the core of the article where the reformulation of the anisotropic